Charge density correlations in t-J ladders investigated by the CORE method

Sylvain Capponi and Didier Poilblanc
Groupe de Physique Théorique, Laboratoire de Physique Quantique, UMR–CNRS 5626
Université Paul Sabatier, F-31062 Toulouse, France[*]
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Using 4-site plaquette or rung basis decomposition, the CORE method is applied to 2-leg and 4-leg t-J ladders and cylinders. Resulting range-2 effective hamiltonians are studied numerically on *periodic rings* taking full advantage of the translation symmetry as well as the drastic reduction of the Hilbert space. We investigate the role of *magnetic* and *fermionic* degrees of freedom. Spin gaps, pair binding energies and charge correlations are computed and compared to available ED and DMRG data for the full Hamiltonian. Strong evidences for *short range* diagonal stripe correlations are found in *periodic* 4-leg t-J ladders.

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Competition between superconducting correlations and charge ordering has long been a challenge to numerical computations [1, 2] of low-dimensional strongly correlated electron systems. Spin and hole-doped ladders [3] offer an ideal system to investigate the cross-over between one to two dimensions. The 2-leg ladder for example is known to exhibit a robust spin gap at and close to half-filling as well as hole pair binding [4, 5]. Dominant power-law $d_{x^2-y^2}$-like pairing and $4k_F$ charge density wave (CDW) correlations at small doping are characteristic of a Luther-Emery (LE) liquid regime [6, 7]. However, the spin gap magnitude drops sharply as the number of legs is increased, e.g. from $0.50\,J$ in the Heisenberg 2-leg ladder to $0.190\,J$ in the Heisenberg 4-leg ladder [8]. Both the increase of the magnetic correlation length (of the undoped ladder) as well as the drastic reduction of the available ladder length for increasing leg number restrict enormously the accuracy of standard numerical techniques like Exact Diagonalisation (ED) and Density Matrix Renormalisation (DMRG) techniques. In addition, the DMRG method is limited (in pratice) to Open Boundary Condition (OBC) in the leg direction.

In this Rapid Communication, we use the Contractor Renormalisation (CORE) method [9, 10] to investigate hole-doped 2-leg and 4-leg ladders [12]. Our aim is to get further insights on the issue of pairing and density correlations from the investigation of large enough systems with *Periodic Boundary Conditions* (PBC) in the ladder direction. Such investigations are greatly needed to complement available DMRG calculations using OBC. Our approach is done in two steps; (i) first, using an appropriate partition into small subsystems, we use the CORE method to construct an effective hamiltonianx which integrates out quantum fluctuations at short length scales; (ii) we use ED techniques (supplemented by finite size analysis) to compute various physical properties (pair binding, spin gaps, etc...) and compare them to those of the original model. The method provides new results such as e.g. strong evidences for stripes correlations in *translationally invariant* 4-leg ladders.

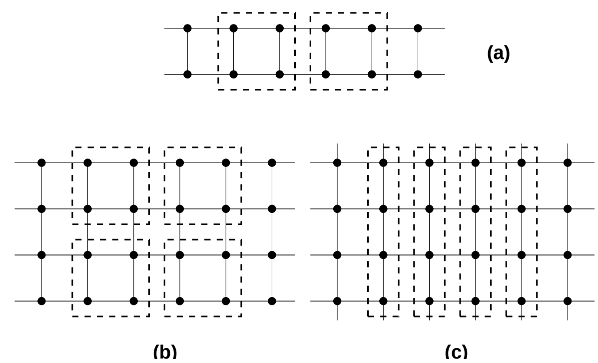

FIG. 1: CORE decomposition in term of plaquette or rung sub-systems; (a) 2-leg ladder split in plaquettes; (b) 4-leg ladder split in 2×2 plaquettes; (c) 4-leg cylinder split in 4-site rungs.

We shall consider here a generic n-leg t-J ladder,

$$\begin{aligned}\mathcal{H} &= J_{\rm leg}\sum_{i,a}\vec{S}_{i,a}\cdot\vec{S}_{i+1,a} + J_{\rm rung}\sum_{i,a}\vec{S}_{i,a}\cdot\vec{S}_{i,a+1} \qquad (1)\\ &+ t_{\rm leg}\sum_{i,a}(c^\dagger_{i,a}c_{i+1,a}+h.c.) + t_{\rm rung}\sum_{i,a}(c^\dagger_{i,a}c_{i,a+1}+h.c.)\,,\end{aligned}$$

where $c_{i,a}$ are projected hole fermionic operators. Open (ladders) or closed systems (cylinders) along the rungs with isotropic coupling, $t_{\rm leg}=t_{\rm rung}=1$ and $J_{\rm leg}=J_{\rm rung}=J$, will be of interest here.

In order to implement the CORE algorithm the ladders are decomposed in small 4-site sub-units as shown in Fig. 1 whose M low-energy states are kept to define a reduced Hilbert space. The full hamiltonian (1) is then diagonalised on N connected units (with OBC) to retain its M^N low-energy states. These true eigenstates are then projected on the reduced Hilbert space (tensorial product of the M states of each unit) and Gram-Schmidt orthonormalized [9, 10]. An effective hamiltonian containing N-body interactions with identical low-energy spectrum can then be constructed in terms of the reduced basis by a unitary transformation [11]. For sake

of simplicity, we shall restrict ourselves to the range-2 approximation($N = 2$) [12].

At half-filling, retaining in each 4-site unit only the lowest singlet and triplet states (4 states) gives excellent results [12]. Away from half-filling, the simplest truncation, referred to as "B" approximation, is to include, in addition, the lowest singlet hole pair on the 4-site unit (of d-wave symmetry in the case of a plaquette). Formally, one can define 4 hard-core bosonic (plaquette or rung) operators describing the 4 possible transitions from the singlet half-filled GS (vacuum) to one component of the triplet state, $t_{\alpha,i}$, or to the hole pair state, b_i (Ref. 13). The effective B-hamiltonian $\mathcal{H}^B$ can then be written as a sum of a simple bilinear kinetic term $\mathcal{H}^b + \mathcal{H}^t$ and a quartic interaction $\mathcal{H}^{int}$ (Refs. 10, 12),

$$\mathcal{H}^b = \epsilon_0 + \epsilon_b \sum_i b_i^\dagger b_i - J_b \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + \text{H.c.} \right) \quad (2)$$

$$\begin{aligned} \mathcal{H}^t &= \epsilon_t \sum_{i\alpha} t_{\alpha i}^\dagger t_{\alpha i} - \frac{J_t}{2} \sum_{\alpha \langle ij \rangle} (t_{\alpha i}^\dagger t_{\alpha j} + \text{H.c.}) \\ &\quad - \frac{J_{tt}}{2} \sum_{\alpha \langle ij \rangle} (t_{\alpha i}^\dagger t_{\alpha j}^\dagger + \text{H.c.}) \,, \end{aligned} \quad (3)$$

$$\begin{aligned} \mathcal{H}^{int} &= V_b \sum_{\langle ij \rangle} n_{bi} n_{bj} + \sum_{\langle ij \rangle} \left[V_0 (t_i t_j)_0^\dagger (t_i t_j)_0 \right. \\ &\quad \left. + V_1 (t_i t_j)_1^\dagger (t_i t_j)_1 + V_2 (t_i t_j)_2^\dagger (t_i t_j)_2 \right] \\ &\quad - J_{bt} \sum_{\langle ij \rangle \alpha} (b_i^\dagger b_j t_{\alpha j}^\dagger t_{\alpha i} + \text{h.c.}) \\ &\quad + V_{bt} \sum_{\langle ij \rangle \alpha} (b_i^\dagger b_i t_{\alpha j}^\dagger t_{\alpha j} + b_j^\dagger b_j t_{\alpha i}^\dagger t_{\alpha i}) \,, \end{aligned} \quad (4)$$

where $(t_i t_j)_S^\dagger$ creates two triplets on plaquettes i and j, which are coupled into total spin S. Such an effective hamiltonian may serve for analytic and numerical treatments. Its parameters listed for $J = 0.35$ and $J = 0.5$ in table I are consistent with those found for the Hubbard model[10]. Although, $\mathcal{H}^B$ gives already a faithful description of the physics of the original model, a systematic improvement can be done by adding to the above local basis 4 extra "fermionic" states corresponding to the degenerate ($S_z = \pm 1/2$, even and odd chirality or parity) single hole GS of the 4-site unit (hereafter referred to as "BF" approximation).

The 2-leg t-J ladder offers an ideal system to test the efficiency of the CORE method and the choice of the plaquette decomposition. As seen from the behavior of the pair-binding energy $\Delta_P = 2E_0(n_h = 1) - E_0(n_h = 2) - E_0(n_h = 0)$ plotted in Fig. 2(a) and from the plaquette charge density-density correlation in the two hole GS of the BF-hamiltonian plotted in Fig 3(a), pairs are found to be strongly bound and localized almost on a single plaquette. This confirms *a posteriori* the relevance of CORE and of the local basis. Furthermore, the finite size scaling of the spin gap for a fixed number of $n_h = 2$ holes

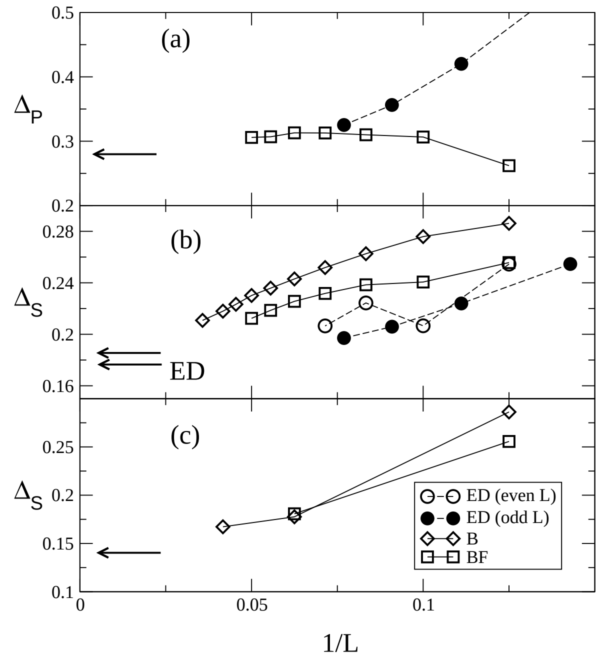

FIG. 2: Finite size scaling analysis vs $1/L$ for a periodic 2-leg $2 \times L$ t-J ladder at $J = 0.5$ using the decomposition of Fig. 1(a) and the effective B- or BF- hamiltonians (as indicated on plot). DMRG & ED data for the original t-J ladder are also shown for comparison. ED data obtained with odd ladder lengths are averaged over boundary conditions (see [18]). DMRG data and $L \to \infty$ ED extrapolations are shown by arrows. (a) Pair-binding energy Δ_P. (b) Spin gap of the 2-hole doped ladder. (c) Spin gap of the 1/8-doped ladder.

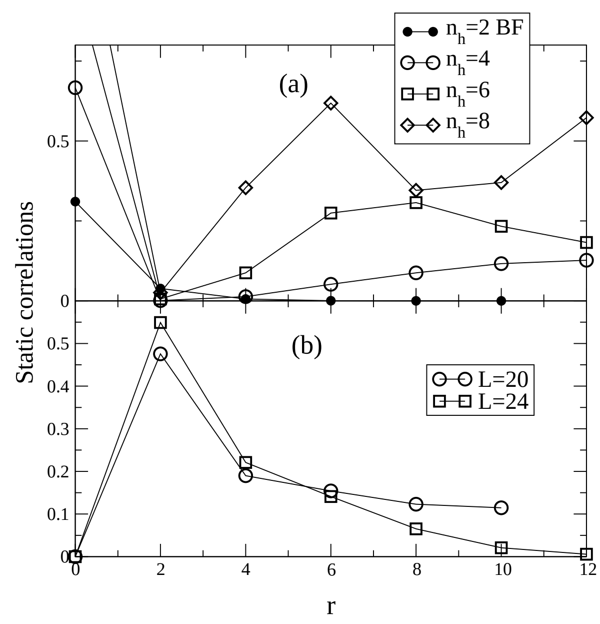

FIG. 3: Correlations as a function of distance (in units of the original bond length) up to $r = L/2$ in $2 \times L$ t-J ladder at $J = 0.5$. (a) Plaquette charge density correlations for $L = 24$. The BF-hamiltonian (B-hamiltonian) is used for $n_h = 2$ holes (otherwise). (b) Hole pair density-S_z correlation in the lowest triplet excited state of 2×20 and 2×24 2 hole-doped ladders using the B-hamiltonian.

J	ϵ_0	ϵ_b	ϵ_t	J_t	J_{tt}	J_b
0.35	-3.8895	-3.5340	0.1379	0.2128	0.2319	0.2139
0.5	-5.5564	-3.0919	0.1970	0.304	0.3112	0.2174
0.35	-3.5564	-3.6579	0.4733	-0.4836	-0.4336	0.4855
J	J_{bt}	V_b	V_0	V_1	V_2	V_{bt}
0.35	-0.0709	1.0345	-0.1244	-0.0928	0.0412	-0.3298
0.5	-0.1044	0.8326	-0.1777	-0.1326	0.0588	-0.3325
0.35	0.2887	1.4164	-0.2158	-0.0202	0.0149	-0.2489

TABLE I: Parameters of $\mathcal{H}^B$ (in units of t) computed for the t-J ladder model using range-2 CORE with 2 plaquettes (row 1 and 2) or 2 4-site rungs (row 3).

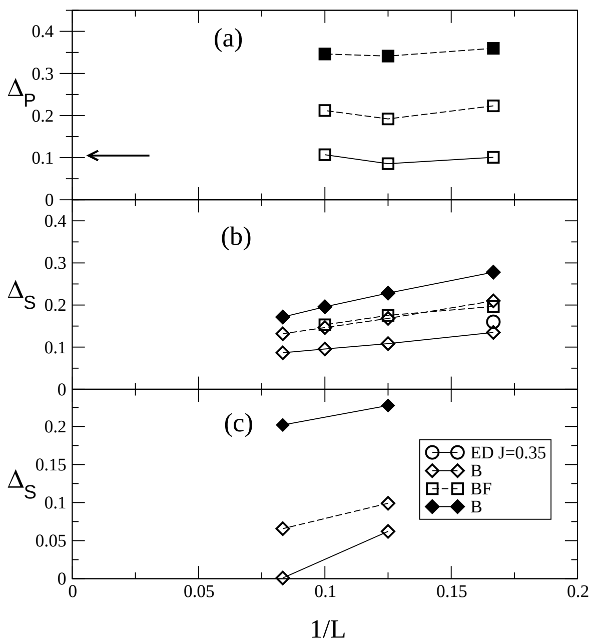

FIG. 4: Finite size scaling analysis vs $1/L$ for a periodic 4-leg $4 \times L$ t-J ladder (open symbols) using the decomposition of Fig. 1(b) for $J = 0.35$ (full lines) and $J = 0.5$ (dashed lines). Data are also shown in the case of a periodic *cylinder* (filled symbols) for $J = 0.35$ using the decomposition of Fig. 1(c). Symbols and notations similar to Figs. 2(a-c). (a) Pair-binding energy Δ_P. (b) Spin gap of the 2-hole doped system. (c) Spin gap of the 1/8-doped system.

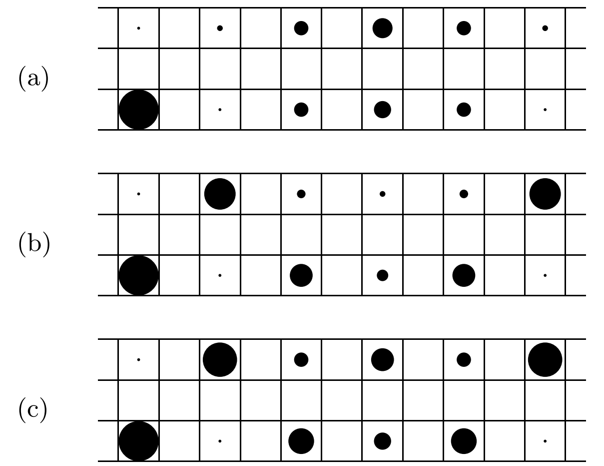

FIG. 5: Hole-pair density-density correlation on a 4×12 ladder at $J/t = 0.35$. PBC are used in the leg direction and correlations are measured from the reference plaquette on the lower left corner. From top to bottom, $n_h = 4, 6, 8$. The surfaces of the dots are proportional to the values of the correlations.

(see Fig. 2(b)) or at 1/8 hole density (Fig. 2(c)) gives gaps with 10-20% accuracy in comparison to existing numerical data [18]. Due to the small size of the hole pairs, accurate results are obtained even when fermionic excitations are not included. Note that the effective models lead to a smooth finite size behavior, in contrast to the original t-J model where "band-filling" effects may lead to oscillatory behaviors as seen in Figs. 2.

We point out the qualitative agreement between our results and those of Siller et al. [17] who used a more involved hard-core charged boson model with longer range repulsive interactions (giving rise to a Luttinger liquid behavior), but neglected both fermionic and gapped triplet excitations [17]. Our more systematic and general treatment using the B-hamiltonian gives a similar qualitative picture as can be seen from the charge correlations shown in Fig.3(a); we observe the characteristic 4k$_F$-CDW spatial oscillations of the LE phase showing the same number of maxima as the number of hole pairs. Let us emphasize that this is also in agreement with DMRG calculations [17]. Our approach performed on finite homogeneous systems is then complementary to the DMRG technique using OBC.

Although the agreement with the hard-core charged boson model is qualitatively good, we believe that including magnetic triplet excitations in the local basis is nevertheless important to describe interplay between magnetic and pairing correlations. For example, it is known that the lowest triplet excitation in a 2 hole doped (or very weakly doped) t-J ladder consists of a hole pair-magnon boundstate [18]. Indeed, the extrapolated value of the spin gap in the presence of 2 holes (see Fig. 2(b)) is lower than that of the undoped ladder ($0.5J$) and than the hole pair binding energy (shown in Fig. 2(a)). Moreover, as seen in Fig.3(b), the correlation between the hole pair density and the plaquette S_z-component clearly shows an enhancement at short distance [14].

We finish the investigation of the 2-leg ladder by using the effective Hamiltonian to calculate the Luttinger liquid parameter K_ρ which governs the long distance power-law behavior of the charge correlations related to the unique massless charge mode. Some values of K_ρ obtained from the Drude weight D and the compressibility κ [15] as $K_\rho = \pi\sqrt{D\kappa/2}$ are listed in table II. In addition, we also list here the charge velocity u_ρ obtained from the relation $u_\rho = \pi D/K_\rho$ and which agrees within a few percents to the values obtained directly from the linear dispersion of the charge mode. Note also that

these values compare very well to existing ED [7] and DMRG [17] data.

doping	14.3%[b]	12.5%[a]	10.7%[b]	8.3%[a]	7.1%[b]	4.2%[a]	3.6%[b]
K_ρ	0.559	0.602	0.668	0.753	0.798	0.914	0.920
u_ρ	0.881	0.779	0.652	0.445	0.399	0.188	0.180

TABLE II: Parameters K_ρ and u_ρ as a function of doping computed on 2×24 (^{a}) and 2×28 (^{b}) ladder with B-hamiltonian and $J/t = 0.5$.

We now turn to the investigation of the 4-leg t-J ladder (with OBC along rungs) or cylinder (with PBC along rungs), for which the best choices of unit decomposition are depicted in Fig. 1(b) and Fig. 1(c) respectively. Results for pair binding energies and spin gaps are shown in Fig. 4(a-c). Results for ladders and cylinders are similar although the hole pair binding is much stronger in cylinders where hole pairs are preferably formed on cross-sectional plaquettes (periodic rungs) rather than on "surface" plaquettes. Generically we found that the pair binding energy is larger than the spin gap of the undoped (Heisenberg) system ($0.190J$ for the $4 \times L$ ladder). Therefore, the lowest triplet state in the 2-hole doped (or very lightly doped) 4-leg ladder is similar to a Heisenberg ladder magnon, which may be (or may not be) loosely bound to a hole pair depending whether its excitation energy is lower or equals the magnon energy of the undoped system. Since the data shown on Fig. 4(b) are not fully conclusive we have computed in addition the hole pair density-S_z correlation and found, as for the 2-leg ladder case, an enhancement of the spin density on the neighboring sites of the hole pair suggesting, indeed, the existence of a hole pair-magnon boundstate.

Upon increasing doping, as seen from the hole-pair density-density correlation shown in Fig.5, we observe a clear tendency of the hole pairs to align along the diagonal $(1, \pm 1)$ directions with a periodicity corresponding to one pair every two plaquettes, a behavior also reported in DMRG calculations[16, 19] and reminiscent of the picture of diagonal stripes. Note that real space charge correlations are fully consistent with the power law decay found in the effective charge boson model [19].

To conclude, the CORE method is a powerful method to extract effective hamiltonians for strongly correlated models. It allows numerical simulations on significantly larger systems than those available for the original model. We show that including charge *and* spin bosonic excitations gives reliable results as long as the hole pair binding energy is not too small. Results for the effective model of the 2-leg t-J ladder are in excellent agreement with known analytic and numerical data. Within the effective models hole pair-triplet bound states form for both 2-leg and 4-leg ladders, a key feature to be compared to $SO(5)$ phenomenological theories[20]. In addition, the method enables unbiased (since calculated on translationnaly invariant clusters) analysis of hole pair density correlations. While $4k_F$-CDW correlations are found in 2-leg ladders, our computations provide clear evidences in favor of short range diagonal stripes in 4-leg ladders.

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* URL: `http://w3-phystheo.ups-tlse.fr`

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[14] Within the 2-site rung decoupling scheme no hole pair-magnon boundstate is found [13] in contradiction with numerical results [18]. However this result might apply to *anisotropic* ladders (J. Riera, private communication).

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